

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 6.26 °C

Global applicability domain: Inside

Local applicability domain index: 6.69e-01

Confidence level: 5.86e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl N-butylcarbamate

Measured: -22.0

Predicted: 56.5

Image not found

1-LAURYL-4-METHOXYCARBONYL-2-PYRROLIDONE

Measured: 27.5

Predicted: 28.6